Closed hierarchies and non-equilibirum steady states of driven systems

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We present a class of tractable non-equilibrium dynamical quantum systems which includes combinations of injection, detection and extraction of particles interspersed by unitary evolution. We show how such operations generate a hierarchy of equations tying lower correlation functions with higher order ones. The hierarchy closes for particular choices of measurements and leads to a rich class of evolutions whose long time behavior can be simulated efficiently. In particular, we use the method to describe the dynamics of current generation through a generalized quantum exclusion process, and exhibit an explicit formula for the long time energy distribution in the limit of weak driving.

Significant activity has been devoted to the study of quantum systems out of equilibrium, with a rapid increase in interest due to the relevance to experiments with ultra-cold atomic gases, whose coherent evolution may be effectively controlled and decoupled from dissipation to a heat bath [1–3]. Non equilibrium dynamics is typically studied in processes such as external driving, repeated quantum measurements and quantum quenches. The fundamental question that arises in such cases is what is the long term behavior of the system: does it eventually reach a non-equilibirum steady state? What is the nature of such a state?

In studying the aforementioned non-equilibrium situations, some highly successful tools of equilibrium statistical physics, such as linear response theory, may easily fail. Thus, there is a need to develop new methods to deal with some of these problems. Here we focus on one such idea - that of establishing closed hierarchies in order to get tractable equations for correlation functions. Specifically, in many statistical mechanics problems, it is possible to make a systematic connection between the evolution of n body density functions with $n+1$ density functions. A prime example for such a set of relations is the Bogoliubov-Born-Green-Kirkwood-Yvon (BBKGY) hierarchy, which is the essential structure leading to the Boltzmann equation. In the Boltzmann equation, single particle densities are tied to higher order correlation functions represented in the collision integral (see, e.g. [4]). In this letter, we describe the requirements on obtaining a hierarchy under general quantum operations on fermions. We then show how the hierarchy may be closed for a quantum system that is periodically evolved, detected, and injected with current. Finally, we use the idea to describe dynamics of current buildup, and the energy distribution in the long term non-equillibirum steady state.

To begin the discussion, consider the most general evolution of a density matrix, describing unitary evolution, measurements and interaction with the environment. Written as

$$\rho \to \mathcal{L}(\rho) = \Sigma_\nu A_\nu \rho A_\nu^\dagger \ ; \ \Sigma_\nu A_\nu^\dagger A_\nu = 1 \tag{1}$$

This form ensures ρ remains a non-negative matrix, and the normalization condition on the Krauss operators A_i ensures that $\mathrm{Tr}\rho = 1$ is preserved under the evolution.

In general, there is no simple relation between correlation functions computed in state ρ before and after the evolution (1), which necessitates working in an exponentially large Hilbert space and is therefore often un-tractable.

Hierarchy structures have been used before in the context of Kossakowski-Lindblad evolution, which is a particular limit of (1). For example, the steady state of a dissipative XX spin chain in the presence of driving and dissipation has been studied extensively [5–8]. Also, conditions for a closed hierarchy in the continuous time frame work where stated in [9]. Here we concentrate on a discrete time framework, but also supply corresponding Kossakowski-Lindblad results in the end as a special limit. In other processes, the possibility of getting a closed equation for Kossakowski-Lindblad evolution of noise averaged expectation values was studied in [10], to explore the stability of fractional charges to noisy hopping processes.

We utilize the power of this approach to study a non-equilibirum process of current generation, as schematically depicted in Fig. 1 (a). In this process, we connect site a to a lead, where a current is injected, and particles are allowed to go out at site b (two choices for b are shown). The process is explicitly described by

$$\begin{aligned}\rho \longrightarrow U((1-r)\rho + r\alpha[a_a^\dagger \rho a_a + n_a \rho n_a] + \\ r(1-\alpha)[a_b \rho a_b^\dagger + (1-n_b)\rho(1-n_b)])U^\dagger,\end{aligned} \tag{2}$$

where $n_{a/b} = a_{a/b}^\dagger a_{a/b}$ checks for the presence of a fermion on the injection/extraction site, and $U = e^{-i\tau \sum h_{nm} a_n^\dagger a_m}$ describes evolution between attempts during a time interval τ. Here r is the overall attempt rate, and α is the relative probability of injecting vs extracting attempts. We show below that this process leads to a closed equation (13) for the two point function of the system, which can be then computed numerically. It is important to emphasize that the long time steady state reached by the system is not a thermal equilibrium state, in that the energy occupation is very different from a Fermi-Dirac distribution governed by h.

For small r, we find a remarkable explicit formula for

the steady state distribution $\Phi_k \equiv \langle steady|a_k^\dagger a_k|steady\rangle$. Here k labels the eigenstates $|k\rangle$ of the single particle hamiltonian h_{nm}, $h|k\rangle = E_k|k\rangle$. Let $p_{a,k} = |\langle a|k\rangle|^2, p_{b,k} = |\langle a|k\rangle|^2$ be overlaps of these states with the sites a, b. Then Φ_k is a function of the ratio $p_{a,k}/p_{b,k}$:

$$\Phi_k = \frac{\mathcal{A} + \mathcal{B}\,\frac{p_{a,k}}{p_{b,k}}}{(1-\alpha) + \alpha\frac{p_{a,k}}{p_{b,k}}} \tag{3}$$

The coefficients $\mathcal{A}, \mathcal{B}$ are given below in Eq. (16). We emphasize that this expression is valid for any system obeying the form (2). The details of the distribution depend of sensitively on the choice of parameters. For illustration, we consider hopping on a chain of length N, with the standard Hamiltonian $H_{hop} = \sum_{i=1}^{N-1} a_i^\dagger a_{i+1} + h.c.$ corresponding to Dirichlet boundary conditions. In this case $p_{a,k}/p_{b,k} = \sin^2(\frac{\pi a k}{N+1})/\sin^2(\frac{\pi b k}{N+1})$. In Fig. 1 we illustrate the result with $N = 100$, and injection at $a = 1$. We evolve the system from an initial vacuum state at $t = 0$. The results for extraction at the final and penultimate sites $b = 100, 99$ respectively, show sensitivity to the choice of operation sites. The energy distribution is computed numerically at long times and is clearly seen to approach Φ in the long time limit. We stress that once driving has stopped, the energy distribution Φ will remain the stationary distribution under the subsequent free evolution.

We now turn to establishing the framework for our processes. We consider a system of fermions on a lattice of N sites. In (1) we take Krauss operators of the form $A_\nu = m_\nu U_\nu$, where U_ν is an evolution under a non-interacting hamiltonian, and m_ν is a polynomial of order r_ν in fermion operators $a^\dagger, a$. The evolution under $\mathcal{L}$ of a general correlation function,

$$\langle a_{i_1}^\dagger..a_{i_k}^\dagger a_{i_{k+1}}..a_{i_{k+l}}\rangle \equiv \mathrm{Tr}\rho a_{i_1}^\dagger...a_{i_k}^\dagger a_{i_{k+1}}...a_{i_{k+l}} \tag{4}$$

is given by

$$\langle a_{i_1}^\dagger..a_{i_k}^\dagger a_{i_{k+1}}..a_{i_{k+l}}\rangle \longrightarrow \langle a_{i_1}^\dagger..a_{i_k}^\dagger a_{i_{k+1}}..a_{i_{k+l}}\rangle + \sum_\nu Tr\ \rho U_\nu^\dagger m_\nu^\dagger [a_{i_1}^\dagger...a_{i_k}^\dagger a_{i_{k+1}}...a_{i_{k+l}}, m_\nu U_\nu] \tag{5}$$

where the normalization relation in (1) was used.

The assumption that the U_ν are non interacting, means that $U_\nu^\dagger a_i U_\nu = u_{\nu;ij} a_j$ for some unitary matrix $u_\nu \in U(N)$. As a consequence the evolution of the $k+l$ correlation function (4), is related in (5) to correlation functions of an order at most $k+l+2\max_\nu(r_\nu)$, establishing a hierarchy of equations.

We emphasize that the resulting state may be arbitrarily complex. Indeed, even when starting with a non-interacting thermal state, $\rho \sim exp(-h_{ij}a_i^\dagger a_j)$ and taking each A_ν a non interacting unitary, ρ evolves into a sum of exponentials of fermion bi-linears. Such a state can be used to approximate any interacting state whose determinant quantum Monte Carlo description does not suffer from a sign problem [11].

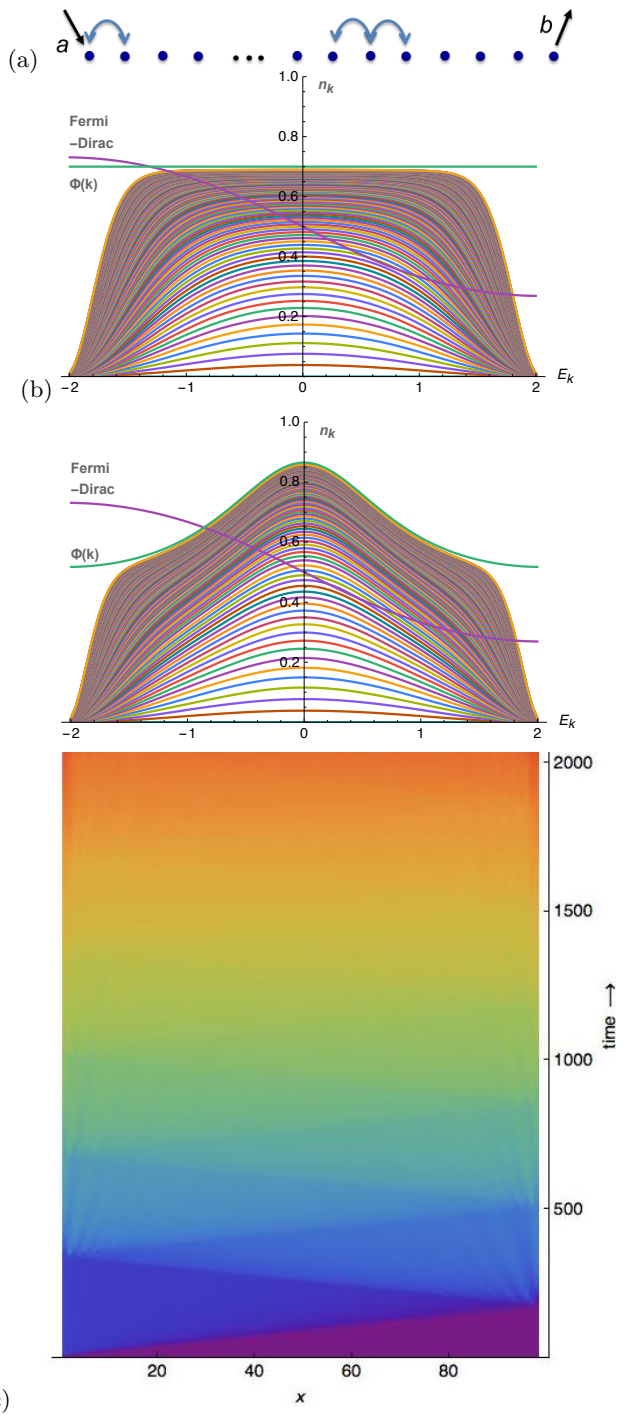

Figure 1: (a) Fermions hopping on a chain. Particles are injected from the left and removed on the right with $r = 0.01, \alpha = 0.7, \tau = 0.1$. (b) Energy occupation approach to $\Phi(n)$. Results for extraction site $b = 100$ (upper panel) and $b = 99$ (lower panel). There are 300 iterations between successive curves. For reference a Fermi-Dirac distribution is also shown. (c) Evolution of the local density, $\langle a_i^\dagger a_i\rangle$, in real space (red/blue corresponds to high/low density).

Below, we list several fundamental operations under which the hierarchy *closes* at the two point function level, for $G_{ij} \equiv \langle a_i^\dagger a_j \rangle$, inducing a map $G \to \mathcal{K}(G)$. We start with the obvious one:

(I) The non-interacting evolution $\mathcal{L}_u(\rho) = U\rho U^\dagger$, as described above, induces a map

$$G_{ij} \to \mathcal{K}_u(G)_{ij} \equiv (u^\dagger G u)_{ij} \tag{6}$$

We augment the free evolution with the following types of operations acting on a single particle mode: particle detection, injection and extraction. Below, for simplicity of presentation we will associate the operation with the mode associated with site i.

Denote P_i the matrix $(P_i)_{r\alpha} = \delta_{ir}\delta_{i\alpha}$ the projection on site i, and $P_i^\perp = 1 - P_i$, we introduce:

(II) Particle detection at site i:

$$\mathcal{L}_{D,i}(\rho) = n_i \rho n_i + (1 - n_i)\rho(1 - n_i) \tag{7}$$

where $n_i = a_i^\dagger a_i$. The induced map on G is:

$$\mathcal{K}_{D,i}(G) = P_i^\perp G P_i^\perp + P_i G P_i \ . \tag{8}$$

The process (II) may be viewed as a "decoherence" of the correlations G in between site i and the rest of the lattice. As a linear super-operator on matrices, the measurement $\mathcal{K}_{D,i}$ has a simple spectrum. It acts as identity on matrices which do not mix site i with the rest, hence the non-zero subspace of matrices has a dimension $1 + (dim P_i^\perp)^2$. The complementary zero subspace is spanned by the off diagonal blocks, of dimensionality $2(dim P_i^\perp)$.

(III) Removal of a particle from site i is described by

$$\mathcal{L}_{out,i}(\rho) = a_i \rho a_i^\dagger + (1 - n_i)\rho(1 - n_i) \tag{9}$$

with the induced map on G:

$$\mathcal{K}_{out,i}(G) = P_i^\perp G P_i^\perp \ . \tag{10}$$

As a super operator this simple map may be viewed as a projection on the space of matrices that do not have an (i, j) or (j, i) element for any j.

(IV) Finally, this operation injects a particle at site i:

$$\mathcal{L}_{in,i}(\rho) = a_i^\dagger \rho a_i + n_i \rho n_i \tag{11}$$

and induces the map

$$\mathcal{K}_{in,i}(G) = P_i + P_i^\perp G P_i^\perp. \tag{12}$$

We note that in contrast with $(I - III)$, the injection $\mathcal{K}_{in,i}$ is an in-homogenuous transformation on matrices, a property which we use below to compute steady states.

We can combine any of the site operations (II-IV) with the unitary evolutions (I) mixing the the addressed site i with the rest of the sites. When no particle injection is present, the particle extraction map will generically drive G to 0, i.e. $(\mathcal{K}_u \mathcal{K}_{Out,i})^n \to 0$ [21]. Similarly, adding particles by injection $(\mathcal{K}_u \mathcal{K}_{In,i})^n$, with no extraction present, will result in $G_{ij} \to \delta_{ij}$, when $n \to \infty$, which is the state where all sites are occupied.

On the other hand the unitary evolution (I) and the detection process (II) preserve the average particle number, i.e. $\langle \sum_i a_i^\dagger a_i \rangle = \mathrm{Tr}\ G$ remains constant under $\mathcal{K}_u, \mathcal{K}_M$.

There are a myriad possible processes described by combinations of the oprations $(I - IV)$. Here we concentrate on current generation processes as described by Eq. (2), involves operations I, III, IV resulting in the map:

$$\begin{aligned} G \to u^\dagger((1 - r)G + r(\alpha P_a^\perp G P_a^\perp + \\ (1 - \alpha)P_b^\perp G P_b^\perp))u + r\alpha u^\dagger P_a u. \end{aligned} \tag{13}$$

This simple model allows for a substantial reduction of complexity from the full quantum problem of describing the evolution of ρ into an evolution equation for the two point function G_{ij}, which can be tractable by either analytical or numerical methods. It is clear at this stage that we can access very interesting situations.

To compute the eventual non-equilibrium steady state for (13) it is convenient to view the transformation on G from a point of view of a super-operator. Here the $N \times N$ matrix G is viewed as an N^2 dimensional vector, and the action of the evolution $\mathcal{L}$ on ρ translates in (13) into:

$$G \to \Lambda G + g, \tag{14}$$

where Λ is an $N^2 \times N^2$ matrix, and g is the inhomogeneous contribution due to the particle injection processes (12), and corresponding to the $r\alpha u^\dagger P_a u$ term in (13).

In general, whenever $g = 0$, the long time behavior will be determined as usual by the largest eigenvectors of Λ. However when $g \neq 0$, the situation is somewhat different: Indeed, from Eq. (14), we see that when $(1 - \Lambda)$ is invertible, there exists a unique stationarity G, that may be written in the form:

$$G_{steady} = (1 - \Lambda)^{-1} g \tag{15}$$

If $\Lambda - 1$ is not invertible, i.e. there are steady states $\Lambda G_r = G_r$, it means that the evolution u has an invariant subspace which does not include the sites a, b. In this case one has to work with a generalized inverse of $(\Lambda - 1)$. A steady solution can either not-exist, or be non-unique of the form $G_{steady} \sim G_r + (1 - \Lambda)^{-1} g$. While inhomogenous equations are a common occurrence in the study of steady states in classical driven systems, they are used less in quantum processes, where evolution is unitary. A recent example of such a non-homogenous equation in a quantum context is the calculation of the expectation values of spin components in the steady state of a spin undergoing periodic laser pulses [12, 13].

In the limit of $r \ll 1$, we were able to solve exactly for the degenerate perturbation theory to lowest order in r,

obtaining for the energy distribution Φ the result (3). While the result may be obtained by a systematic calculation, it is rather lengthy, and instead here we simply state it as an anzats, which can be explicitly checked by the reader: taking $G = \sum_k \Phi_k |k\rangle\langle k| + rD$, where D is an off diagonal matrix, and plugging into (13) one can verify that Φ is stationary under (13) to leading order in r. Some details of the derivation are supplied in the supplementary material. The coefficients are given by certain overlaps. Define:

$$\mu_l = 2\left(\alpha p_{a,l} + (1-\alpha)p_{b,l}\right) \; ; \; Q_{st} = \Sigma_l \frac{p_{s,l}p_{t,l}}{\mu_l} \; , \; s,t \in \{a,b\}$$

Then $\mathcal{A}, \mathcal{B}$ in (3) are given by

$$\mathcal{A} = \frac{\alpha(1-\alpha)Q_{ab}}{\mu} \; ; \; \mathcal{B} = \frac{\alpha\left(1-(1-\alpha)Q_{bb}\right)}{\mu} \qquad (16)$$

where

$$\mu = 2(1-\alpha Q_{aa} - (1-\alpha)Q_{bb} + \alpha(1-\alpha)(Q_{aa}Q_{bb} - {Q_{ab}}^2))$$

the form of the off-diagonal part D can also be obtained. We have verified the validity of the result numerically on numerous cases in addition to the one depicted in Fig. 1(b). We see that to leading order, Φ is independent of r. How can we understand this? Note that at $r = 0$, there are infinitely many steady states (any G such that $[G, h] = 0$). However, when $r \neq 0$, Λ stops being degenerate and it singles out a particular direction of breaking the degenerate space of matrices.

The dependence of the dynamics on the initial condition is of interest by itself. While in Fig. 1, we started the evolution from the vacuum state, in Fig. 2, we describe such a process where the system is started off as the ground state of H_{hop}. The evolution happens in stages. In the initial stage of evolution we observe two shock wave fronts: one propagating with a region of reduced density from the right, collides with a front of enhanced density propagated from the left. It is interesting to note that the evolution is on a faster time scale than the speed of propagation of a wave-packet localized at a point by free evolution. In the context of classical non equilibrium processes, shock waves have been described for the asymmetric exclusion process in e.g.[14] (It is possible to use the present system also to describe such situations, however this will be done elsewhere).

As the fronts collide the imbalance between the left and right sides of the chain starts to decrease. Finally, soliton like density packets of different velocities, are observed at longer time scales, and may be related to the soliton described in [15] in the context of the orthogonality catastrophe. It is interesting to note the injected particles traveling from the left travel with faster velocities compared to their partners from the other side.

In Fig. 2 we show the average particle density $\bar{n} \equiv N^{-1}TrG$. One of the interesting features observed is

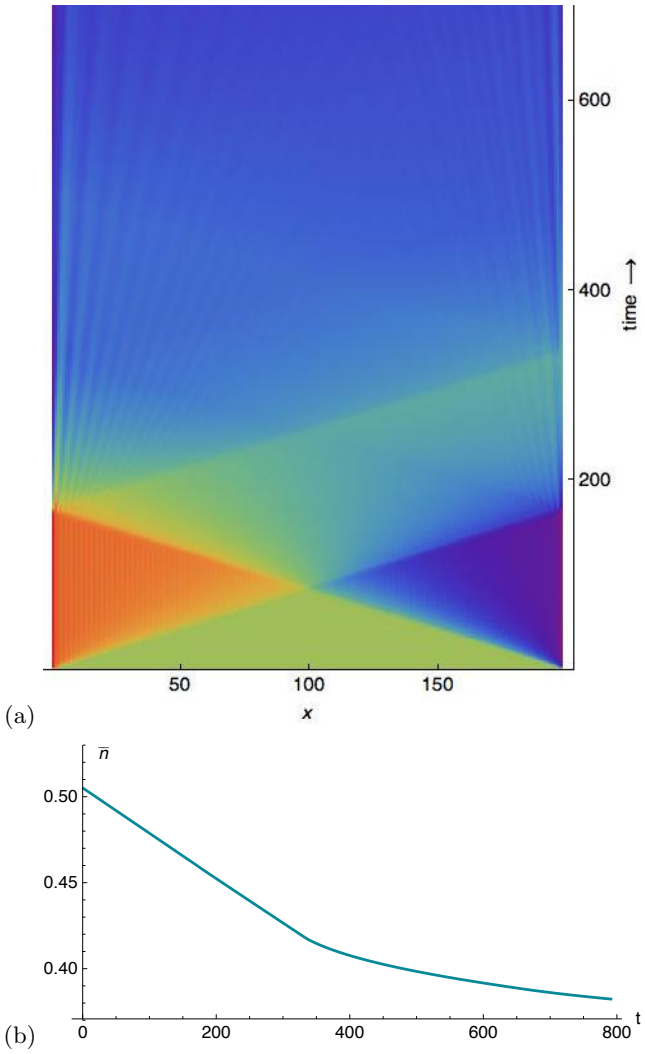

Figure 2: Density depletion in a system where particles are extracted from the right at higher rate than injected on the left, here $r = 1$ and $\alpha = 0.3$, initial state is the half filled ground state of H_{hop}. (a) Real space evolution of local density. (b) Evolution of space averaged density.

a qualitative change in the slope of $\bar{n}(t)$ around 350 iterations. This change seems to correspond to the annihilation of the high density front coming from the left. To check this behavior, we consider, in Fig. 3 the evolution when the initial stage is asymmetric itself: Here in the initial stage all sites i on the left, $i < 100$, are empty, while all sites on the right $i > 100$ are occupied. This state evolves through four fronts that collide and eventually annihilate. Note that for coherent evolution from such an initial state, it has been shown that the front propagation has a scaling $1/t^3$ [16]. In the context of evolution of magnetization in a spin chain the evolution of initial domain wall was studied in [17].

Comparing the density evolution in Fig. 2 and Fig. 3, we see that there is a transient behavior associated with the different nature of the initial states, and their stages of

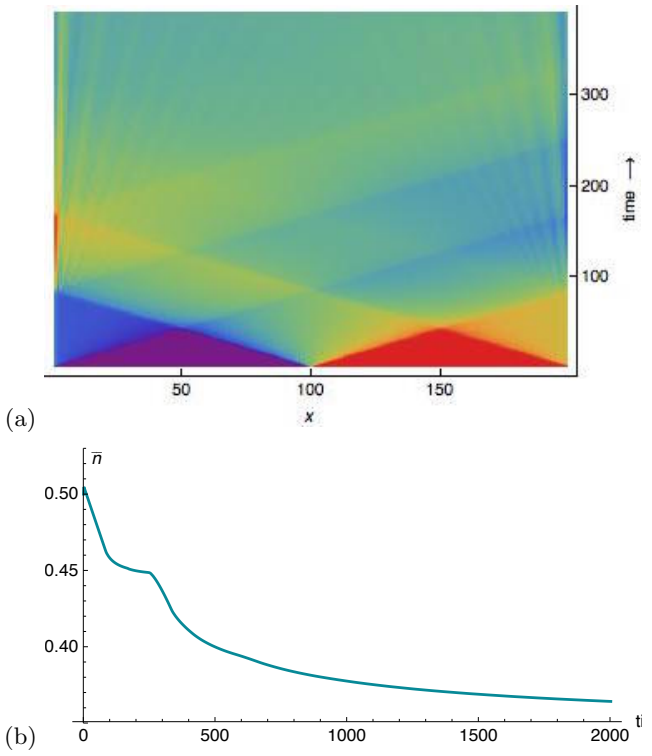

Figure 3: (a,b) Density evolution under the same dynamics as Fig. 2, however with a domain wall as an initial state. Here the depletion happens in two steps, but eventually reaches the same asymptotic value ($\bar{n} \sim 0.38$) as for the initial uniform case.

evolution. In Fig. 3, there is a noticeable change in depletion rate around 100 and 300 iterations, the first kink corresponds the initial high density region on the right hitting the left side: at that point injection of particles becomes harder for a while and $|\partial_t \bar{n}|$ decreases until the density goes down enough on the left. The second kink is observed when the high density region is reflected back to the right: extracting particles on the right is then easier and $|\partial_t \bar{n}|$ grows. At long times the density seems to decay asymptotically as $1/t$ towards the non-equilibrium steady state density.

Finally, we consider the Kossakowski-Lindblad limit, whose treatment is considerably simpler. Starting with:

$$\dot{\rho} = \frac{1}{i\hbar}[H,\rho] + \gamma_a(a_a^\dagger \rho a_a - \frac{\{\rho, a_a a_a^\dagger\}}{2}) + \gamma_b(a_b \rho a_b^\dagger - \frac{\{\rho, a_b^\dagger a_b\}}{2})$$

the equation for G is:

$$\dot{G} = -\frac{i}{\hbar}[G,h^t] - \{\frac{\gamma_a P_a + \gamma_b P_b}{2}, G\} + \gamma_a P_a. \qquad (17)$$

For $\gamma_{a,b} \ll 1$ the steady state, $\dot{G} = 0$, we find:

$$\Phi_k \equiv \frac{\gamma_a p_{a,k}}{\gamma_a p_{a,k} + \gamma_b p_{b,k}}. \qquad (18)$$

This last expression has a simple interpretation: the probability of occupying a given energy level is determined by the ratio between the effective tunneling probability into energy k from site a compared to the effective tunneling rate of the state k through site b.

Summary: We presented a class of non equilibrium quantum processes that correspond to closed hierarchies of evolution equations, and can thus be studied numerically efficiently. We have used this idea to explore non-equllibrium generation of currents and approach to steady states. We remark that the resulting states may also be viewed as Floquet states, and we have thus supplied a particular way of engineering such states, that may be of interest in the context of topological Floquet states[18–20]. Moreover, the energy distribution Φ_k should be studied further: one can hope to test the resulting highly excited current carrying steady states in a variety of settings from cold atoms to mesoscopic systems and spin chains. We emphasize that our result does not rely on integrability that has been used in studies of dissipative spin chains, and is available for periodically driven fermion systems that do not correspond to spin chains, including higher dimensional systems.

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[21] The limit $G \to 0$ is not at odds with the validity of the map $\mathcal{L}$ at the level of density matrices: acting on density matrices $\mathcal{L}$ has to be positive and trace preserving. Here, the limit $G \to 0$ simply means $\rho \to |vac\rangle\langle vac|$ where the vacuum state $|vac\rangle$ is a perfectly normalizable state with $G = 0$.

Supplementary Material

In this section we derive the formulas (3,16) for the energy distribution Φ.

We study the steady state equation associated with the process (13):

$$G_{steady} = (1-r)\ u^\dagger G_{steady} u + \\ u^\dagger r\alpha(P_a + P_{a\perp} G_{steady} P_{a\perp})u + \\ u^\dagger r(1-\alpha)(P_{b\perp} G_{steady} P_{b\perp})u \tag{19}$$

where $u = e^{-i\tau h_0}$.

Below we label the eigenstates of h_0 by n, $h_0|n\rangle = E_n|n\rangle$, and would like to find the probability to find a state with energy E_n occupied in the steady state. This probability is given by $\Phi_n \equiv Tr(\rho a_n^\dagger a_n) = \langle n|G|n\rangle$.

For $r = 0$, all states where $[G, h] = 0$, are immediately invariant under time evolution. Therefore, in the limit of $r \ll 1$ we look for an ansatz for the steady state G_{steady} which is approximately diagonal. Let us write, in the energy basis, the ansatz:

$$G_{steady} = \mathrm{diag}(\{\Phi_1, ...\}) + rD, \tag{20}$$

where $\Phi_n = \langle n|G_{steady}|n\rangle$ are the steady states occupations, and D is an off-diagonal matrix in energy space. Eq. (19) becomes:

$$\Phi + rD = (1-r)\Phi + (1-r)ru^\dagger D u + r\alpha u^\dagger P_a u + \\ r\alpha u^\dagger(P_{a\perp}\Phi P_{a\perp})u + u^\dagger r(1-\alpha)(P_{b\perp}\Phi P_{b\perp})u + O(r^2) \tag{21}$$

We note that the zeroth order is eliminated and we wind up with:

$$D = -\Phi + u^\dagger D u + \\ \alpha u^\dagger P_a u + \alpha u^\dagger(P_{a\perp}\Phi P_{a\perp})u + u^\dagger(1-\alpha)(P_{b\perp}\Phi P_{b\perp})u \tag{22}$$

Furthermore, note that both $D, u^\dagger D u$ are off-diagonal in energy. Therefore we have a closed equation for the diagonal elements:

$$0 = -\Phi_n + \alpha P_{a,\mathrm{nn}} + \\ \alpha(P_{a\perp}\Phi P_{a\perp})_{\mathrm{nn}} + (1-\alpha)(P_{b\perp}\Phi P_{b\perp})_{\mathrm{nn}}. \tag{23}$$

Next, we write:

$$(P_{a\perp}\Phi P_{a\perp})_{\mathrm{nn}} = (\Phi - P_a\Phi - \Phi P_a + P_a\Phi P_a)_{\mathrm{nn}} = \\ \Phi_n - 2P_{a,\mathrm{nn}}\Phi_n + \Sigma_l P_{a,\mathrm{nl}}\Phi_l P_{a,\mathrm{ln}} \tag{24}$$

and we write (23) as:

$$0 = \alpha P_{a,\mathrm{nn}} - \Phi_n(\alpha P_{a,\mathrm{nn}} + (1-\alpha)P_{b,\mathrm{nn}}) \\ +\Sigma_l(\Phi_l - \Phi_n)(\alpha P_{a,\mathrm{nl}}P_{a,\mathrm{ln}} + (1-\alpha)P_{b,\mathrm{nl}}P_{b,\mathrm{ln}}) \tag{25}$$

where we also used:

$$\Sigma_l P_{a,\mathrm{nl}}P_{a,\mathrm{ln}} = P_{a,\mathrm{nn}} \tag{26}$$

At this point it is possible to argue that:

$$|\Sigma_l(\Phi_l - \Phi_n)(\alpha P_{a,\mathrm{nl}}P_{a,\mathrm{ln}} + (1-\alpha)P_{b,\mathrm{nl}}P_{b,\mathrm{ln}})| \tag{27}$$

is small, giving us a first guess for the answer:

$$\Phi_n \sim \frac{\alpha P_{a,\mathrm{nn}}}{\alpha\ P_{a,\mathrm{nn}} + (1-\alpha)P_{b,\mathrm{nn}}} \tag{28}$$

However, it is possible to do better and solve equation (23) exactly.

To do so we write:

$$P_{a,\mathrm{nl}} = \langle n, a\rangle\langle a, l\rangle \equiv f(n)f^*(l)\ ; \\ P_{b,\mathrm{nl}} = \langle n, b\rangle\langle b, l\rangle \equiv g(n)g^*(l) \tag{29}$$

Going back to (23) we write it as:

$$0 = \alpha P_{a,\mathrm{nn}} - 2\Phi_n(\alpha P_{a,\mathrm{nn}} + (1-\alpha)P_{b,\mathrm{nn}}) + \\ \Sigma_l\Phi_l(\alpha P_{a,\mathrm{nl}}P_{a,\mathrm{ln}} + (1-\alpha)P_{b,\mathrm{nl}}P_{b,\mathrm{ln}}) \tag{30}$$

This equation becomes:

$$0 = \alpha|f_n|^2 - 2\Phi_n(\alpha|f_n|^2 + (1-\alpha)|g_n|^2) + \\ \Sigma_l\Phi_l(\alpha|f_n|^2|f_l|^2 + (1-\alpha)|g_n|^2|g_l|^2) \tag{31}$$

We rewrite the equation as a in-homogenous linear equation:

$$\mathcal{Q}^2\vec{\Phi} = \alpha Z_F\vec{F} + V\vec{\Phi}. \tag{32}$$

Here $\vec{F}$ is a unit vector defined by:

$$\vec{F} = \frac{|f_n|^2}{Z_F} \quad ; \quad Z_F = \sqrt{\Sigma_n|f_n|^4}, \tag{33}$$

$\mathcal{Q}$ is a diagonal matrix

$$\mathcal{Q}_{\mathrm{nm}} = \delta_{\mathrm{nm}}\sqrt{\mu_n}\ ;\ \mu_n = 2(\alpha\ |f_n|^2 + (1-\alpha)|g_n|^2), \tag{34}$$

and V can be written in the form

$$V_{\mathrm{nm}} = \alpha|f_n|^2|f_m|^2 + (1-\alpha)|g_n|^2|g_m|^2 = \\ \alpha Z_F^2|F\rangle\langle F| + (1-\alpha)Z_G^2|G\rangle\langle G|. \tag{35}$$

The solution is given formally by:

$$(\mathcal{Q}^2 - V)\vec{\Phi} = \alpha Z_F \vec{F} \Longrightarrow \quad (36)$$
$$\vec{\Phi} = \frac{1}{\mathcal{Q}^2 - V}\alpha Z_F \vec{F} = \alpha Z_F \mathcal{Q}^{-1}\frac{1}{1-\mathcal{Q}^{-1}V\mathcal{Q}^{-1}}\mathcal{Q}^{-1}\vec{F}.$$

Next, we define the unit vector $|F_Q\rangle$ as

$$|F_Q\rangle = Z_{\rm FQ}^{-1}\mathcal{Q}^{-1}|F\rangle. \quad (37)$$

We see that:

$$\langle n|F_Q\rangle = \frac{1}{Z_{\rm FQ}}\frac{1}{\sqrt{\mu_n}}\frac{|f_n|^2}{Z_F}, \quad (38)$$

with the normalization

$$Z_{\rm FQ}^2 = \Sigma_n \frac{|f_n|^4}{\mu_n Z_F^2} \ ; \ \|F_Q\|^2 = 1. \quad (39)$$

Similarly we have

$$(\mathcal{Q}^{-1}|G\rangle)_n = \frac{1}{\sqrt{\mu_n}}\frac{|g_n|^2}{Z_G} = Z_{\rm GQ}|G_Q\rangle; \ Z_{\rm GQ}^2 = \Sigma_n \frac{|g_n|^4}{\mu_n Z_G^2}.$$

Using these, (36) is expressed as:

$$\vec{\Phi} = \quad (40)$$
$$\alpha\mathcal{Q}^{-1}\left(\frac{Z_F Z_{\rm FQ}}{1-\alpha Z_F^2 Z_{\rm FQ}^2|F_Q\rangle\langle F_Q| - (1-\alpha)Z_G^2 Z_{\rm GQ}^2|G_Q\rangle\langle G_Q|}\right)|F_Q\rangle$$

In the next step we use the following relation:

$$\frac{1}{1+a|v\rangle\langle v|+b|u\rangle\langle u|}|v\rangle = \quad (41)$$
$$\frac{1}{1+a+b+ab(1-|\langle v,u\rangle|^2)}\{(1+b)|v\rangle - b\langle u,v\rangle|u\rangle\},$$

which holds for normalized vectors $||u|| = ||v|| = 1$. We are not aware if the expression (41) appears in the literature, but it can be verified explicitly by multiplying both sides by $(1 + a|v\rangle\langle v| + b|u\rangle\langle u|)$.

We will use (41) on (40), with $|F_Q\rangle, |G_Q\rangle$ playing the role of $|u\rangle, |v\rangle$. Thus, we take in (41):

$$a \to -\alpha Z_F^2 Z_{\rm FQ}^2 \quad ; \quad b \to -(1-\alpha)Z_G^2 Z_{\rm GQ}^2, \quad (42)$$

and we also need

$$c \equiv \langle F_Q|G_Q\rangle = \Sigma_n \frac{1}{Z_G Z_F Z_{\rm FQ} Z_{\rm GQ}}\frac{|g_n|^2|f_n|^2}{\mu_n} = \quad (43)$$
$$\frac{1}{Z_G Z_F Z_{\rm FQ} Z_{\rm GQ}}\Sigma_n \frac{|g_n|^2|f_n|^2}{\mu_n}$$

noting

$$Z_F Z_{\rm FQ} = \sqrt{\Sigma_n \frac{|f_n|^4}{\mu_n}} \ ; \ Z_G Z_{\rm GQ} = \sqrt{\Sigma_n \frac{|g_n|^4}{\mu_n}} \quad (44)$$

we have

$$c = \frac{1}{\sqrt{(\Sigma_l \frac{|f_l|^4}{\mu_l})(\Sigma_l \frac{|g_l|^4}{\mu_l})}}\Sigma_n \frac{|g_n|^2|f_n|^2}{\mu_n} \quad (45)$$

Using these expressions with (41) and (40) we find:

$$\Phi_n = \frac{\alpha Z_F Z_{\rm FQ}}{\sqrt{\mu_n}}\left(\left(\frac{1}{1-\alpha Z_F^2 Z_{\rm FQ}^2|F_Q\rangle\langle F_Q| - (1-\alpha)Z_G^2 Z_{\rm GQ}^2|G_Q\rangle\langle G_Q|}\right)|F_Q\rangle\right)_n =$$
$$\frac{\alpha Z_F Z_{\rm FQ}}{\sqrt{\mu_n}}\frac{1}{1-\alpha Z_F^2 Z_{\rm FQ}^2 - \beta Z_G^2 Z_{\rm GQ}^2 + \alpha Z_F^2 Z_{\rm FQ}^2 \beta Z_G^2 Z_{\rm GQ}^2(1-|c|^2)} \times$$
$$\{(1-\beta Z_G^2 Z_{\rm GQ}^2)\langle n|F_Q\rangle + \beta Z_G^2 Z_{\rm GQ}^2 c^*\langle n|G_Q\rangle\} =$$
$$\frac{\alpha}{\mu_n}\frac{(1-\beta Z_G^2 Z_{\rm GQ}^2)|f_n|^2 + \beta Z_F Z_{\rm FQ} Z_G Z_{\rm GQ} c^* |g_n|^2}{1-\alpha Z_F^2 Z_{\rm FQ}^2 - \beta Z_G^2 Z_{\rm GQ}^2 + \alpha Z_F^2 Z_{\rm FQ}^2 \beta Z_G^2 Z_{\rm GQ}^2(1-|c|^2)}.$$

Explicitly:

$$\Phi_n =$$
$$\frac{\mu_n^{-1}\alpha[(1-(1-\alpha)(\Sigma_l \frac{|g_l|^4}{\mu_l}))|f_n|^2 + (1-\alpha)(\Sigma_l \frac{|g_l|^2|f_l|^2}{\mu_l})|g_n|^2]}{1-\alpha(\Sigma_l \frac{|f_l|^4}{\mu_l}) - (1-\alpha)(\Sigma_l \frac{|g_l|^4}{\mu_l}) + \alpha(1-\alpha)((\Sigma_l \frac{|f_l|^4}{\mu_l})(\Sigma_l \frac{|g_l|^4}{\mu_l}) - (\Sigma_l \frac{|g_l|^2|f_l|^2}{\mu_l})^2)}$$

so that:

$$\Phi_n = \frac{\alpha}{\mu_n}\frac{(1-(1-\alpha)Q_{\rm bb})|f_n|^2 + (1-\alpha)Q_{\rm ba}|g_n|^2}{1-\alpha Q_{\rm aa} - (1-\alpha)Q_{\rm bb} + \alpha(1-\alpha)(Q_{\rm aa}Q_{\rm bb} - {Q_{\rm ba}}^2)} \quad (46)$$

with

$$Q_{\rm aa} = \Sigma_l \frac{|f_l|^4}{\mu_l} \ ; \ Q_{\rm bb} = \Sigma_l \frac{|g_l|^4}{\mu_l} \ ; \ Q_{\rm ba} = \Sigma_l \frac{|f_l g_l|^2}{\mu_l}, \quad (47)$$

which is the energy distribution formulas (3,16) in the paper.